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Conference title

Signal Processing in Portable Ion Mobility Spectroscopy

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Abstract

Ion mobility spectroscopy (IMS) is an analytical technique based on multi-disciplinary such as analytical chemistry, electronics, nuclear technique, etc. It is used to separate and identify ionized molecules in the gas phase based on their ion mobility in a carrier buffer gas. In recent years, explosives and drugs become an increasing security risk. Ion mobility spectroscopy (IMS) is a sensitive and low cost device that very suits for explosives and drugs detection, especially in the rapid field detection. We implemented the whole system on a dual-core board including a digital signal processor (DSP) and a microcontroller unit (MCU) for a home-made IMS instrument. Since the ion mobility spectroscopy (IMS) outputting signal is highly introduced with noise and background signals, fast signal processing to separate the spectrum signal from big noise and to locate the peaks in such an embedded system is the most important work for meeting the real-time field detecting requirement. In this paper, the signal acquisition, control and data processing such as digital filtering, de-noising, background subtraction, peak searching are discussed in details. Experimental results show that all true peaks were accurately located from high noised spectrum, and whole circle processing time was less than 25ms, well satisfied system real-time requirement of 30ms recurrence time.

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Keywords: Ion Mobility Spectrometry (IMS), Digital Signal Controller (DSC), Discrete Cosine Transformation (DCT), Background Subtraction, Peak Searching

1. INTRODUCTION

Ion mobility spectroscopy (IMS) is a rugged, portable, sensitive, low cost, field instrumental technique capable of trace organic detection and monitoring for environmental pollutants, pesticides, explosives, narcotics, and other analytes [1][2]. The IMS includes two parts: the detector system and signal processing & control system.

The schematic diagram of an IMS detector device is given in Figure 1, the detector includes four components: ion source region, ion gate, drift region and a detector [2]. The ionized samples from the sample inlet are ionized by the ionizing source. The ionized species are separated in the drift tube by their mobilities in the electric field at atmosphere pressure. Mobilities are mainly based on the size, shape, mass and charges of the ionized species. Ion current is measured by the collector electrode to result a spectrum. Sample analytes can be identified from the

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acquired spectrum. Ionizing sources can be chosen, according to the field of practices, from radioactive source, photo ionization, laser ionization, surface ionization or electro spray. Here we use a radioactive ^{63}Ni (beta emitter).

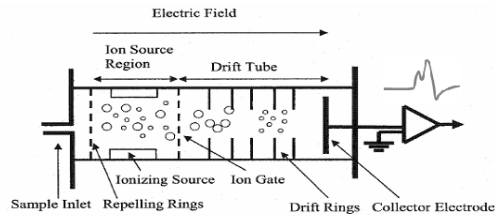


Fig. 1. The schematic diagram of IMS

The signal processing and control part can be realized by a general computer plus a multi-functional signal processing board to build a desktop platform [3][4]. Here we concentrated on DSP based portable platform.

Since the noise and background signal are introduced, detector output signal is the mixture of detecting signal and the noise-background signal, all real-time procedures such as ADC signal acquisition, filtering, de-noising, background subtraction, peaks searching and positioning, etc, must be implemented on the DSP effectively. The ion mobility is heavily related with the gas velocity and temperature in the drift region, feedback control of these parameters is compulsory to the IMS system. We bring in DSP-based embedded subsystem to match the signal process and feedback control requirement, and enhance this system with real-time monitoring capability. Figure 2 gives the diagram of this system.

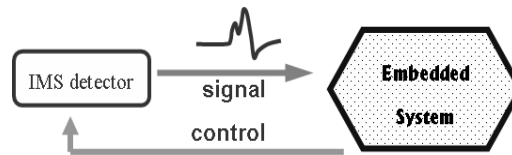


Fig. 2. The diagram of IMS system

2. THE STRUCTURE OF THE IMS SYSTEM

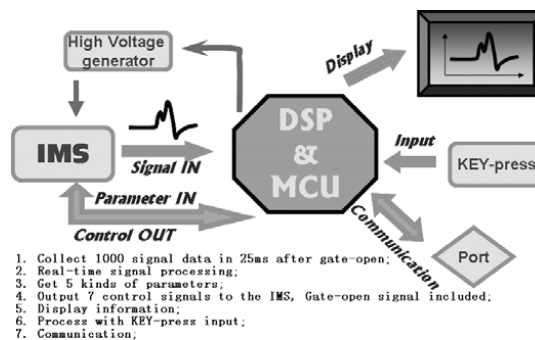


Fig. 3. IMS system requirement and structure

As we mentioned above, the IMS system include two parts: the detector device and the embedded control system. The control system is composed of the DSP and MCU (ARM-core) chips. The DSP chip is deployed for signal

processing while the MCU chip is used for user interface (UI) and communication. In our system, the two points' gas velocities and three points' temperatures need to be acquired with the DSP, (see Figure 4), feed-back control in closed loop with the PID algorithm, high-voltage generation and ion gate opening signal are also processed by the TMS320F28335, a float-point Digital Signal Controller (DSC) and Processor released by Texas Instruments.

The IMS detector output signal requires 1000 samplings at the rate of 40 kHz for every 30 ms after the ion gate opened, followed by filtering, de-noising, background subtraction and peaks seeking of the spectrum as the Figure 5 shows.

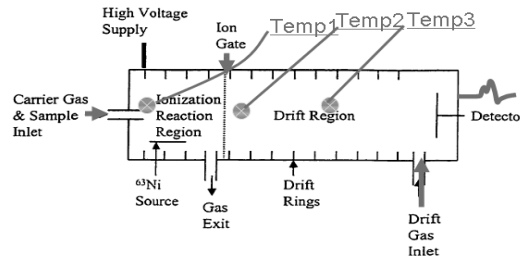


Fig. 4. The diagram of IMS detector device

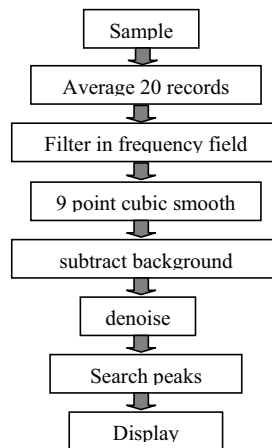


Fig. 5. The flow chart of IMS signal processing

3. SIGNAL ACQUISITION WITH TI F28335

The F2833x/F2823x devices include an enhanced ADC module [5]. The ADC interface is built around a fast, 12-bit ADC module with a fast conversion rate of up to 80 ns at 25-MHz ADC clock. The ADC module has 16 channels, configurable as two independent 8-channel modules. The two independent 8-channel modules can be cascaded to form a 16-channel module. Although there are multiple input channels and two sequencers, there is only one converter in the ADC module. Figure 6 shows the block diagram of the ADC module.

The two 8-channel modules have the capability to auto-sequence a series of conversions. Each module has the choice of selecting any one of the respective eight channels available through an analog MUX. In the cascaded mode, the auto-sequencer functions as a single 16-channel sequencer. On each sequencer, once the conversion is complete, the selected channel value is stored in its respective RESULT register.

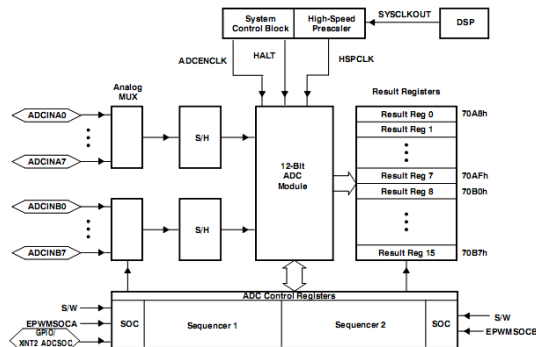


Fig. 6. Block diagram of the ADC module in 28335 DSP

Here we use ‘Sequencer1’ to acquire the IMS ion signal for 1000 sampling data at every 30 ms after the ion gate opened, with a 40kHz sample-rate. ‘Sequencer2’ is used to acquire 5 channels of IMS device status signals that include the Gas velocities and temperature information in the IMS detector device at the rate of 1 sample per minute. The internal ‘timer1’ generate an interrupt signal in every 30ms and the internal ‘timer2’ generate an interrupt signal in every 1 minute. In ‘timer1’s ISR, we check the SEQ1_Busy and SEQ2_busy signals, if the ADC is converting, keep waiting until the ADC is in IDLE state. Then initialize the DMA module and set the SOC1 signal and the ADC will start to convert the IMS ion signal automatically.

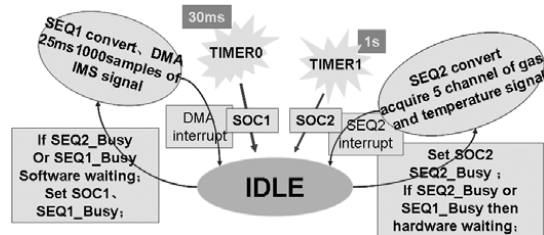


Fig. 7. Signal acquisition in IMS system

The data will be transferred and saved by the DMA without any CPU’s work. This converting takes 25ms. After 1000 sampling data is collected there will be an interrupt by DMA module, then reset SEQ1_busy and ADC module returns IDLE. And in timer2’s ISR we only check the signal SEQ2_busy, if the ADC is not converting ‘Sequencer2’ (1 sample of Gas velocity and temperature information per minute), set the SOC2 signal, and the ADC hardware itself will wait until the ‘Sequencer1’ stopping to start ‘Sequencer2’s converting. This converting takes 125us and ended by the ‘Sequencer2’s interrupt. The IMS ion signal converting takes much more time whilst hardware waiting can largely save the CPU resources, therefore, the software waiting is used to start IMS ion signal converting while hardware waiting is applied to start IMS device status information signals converting. However the IMS device status information signals converting takes much fewer time and software wait can be easily to set the DMA module’s parameters.

By now, both the IMS ion signal and device status information signals are sampled and converted.

4. IMS signal preprocessing by TI F28335

IMS signal is interfused with the background signal and the noise. Simple, fast but effective processing steps including data averaging, filtering, smoothness, background subtracting and de-noise, need to be taken before the peak searching.

4.1. DCT and Filter in frequency domain

Here we use a fast 2^n length DCT algorithm to implement frequency field filter [6] [7]. For an N length sequence signal $\{x(n); n = 0, 1, \dots, N-1\}$ (here $N=1024$), as DCT defined:

$$X(k) = \alpha(k) \sum_{n=0}^{N-1} x(n) \cdot \cos \frac{2\pi}{4N} k(2n+1); \quad k = 0, 1, \dots, N-1 \quad (1)$$

$$\text{Here, } \alpha(k) = \begin{cases} 1/\sqrt{2} & k=0 \\ 1 & k \neq 0 \end{cases}$$

To make the discussion easily understandable, we ignore this factor in the following discussion.

For even subscript- $X(2k)$, we make up an expression

$$u(n) = x(n) + x(N-1-n), \quad n = 0, 1, \dots, \frac{N}{2}-1 \quad (2)$$

Then,

$$U(k) = X(2k) = \sum_{n=0}^{\frac{N}{2}-1} u(n) \cos \frac{2\pi}{2N} k(2n+1) \quad (3)$$

$$k = 0, 1, \dots, \frac{N}{2}-1$$

Therefore, the $X(2k)$ can be obtained from an $N/2$ length DCT result $U(k)$.

In the same way, for odd subscript- $X(2k+1)$, we have the expression as below:

$$v'(n) = x(n) - x(N-1-n), \quad n = 0, 1, \dots, \frac{N}{2}-1 \quad (4)$$

$$X(2k+1) = \sum_{n=0}^{\frac{N}{2}-1} v'(n) \cos \frac{2\pi}{4N} (2k+1)(2n+1) \quad k = 0, 1, \dots, \frac{N}{2}-1 \quad (5)$$

$$X(1) = \frac{1}{2} \sum_{n=0}^{\frac{N}{2}-1} [2v'(n) \cos \frac{2\pi}{4N} (2n+1)] \quad (6)$$

$$\begin{aligned} & X(2k+1) + X(2k-1) \\ &= \sum_{n=0}^{\frac{N}{2}-1} [2v'(n) \cos \frac{2\pi}{4N} (2n+1)] \cos \frac{2\pi}{2N} k(2n+1) \quad (7) \\ & \quad k = 1, \dots, \frac{N}{2}-1 \end{aligned}$$

Let:

$$v(n) = v'(n) \cdot 2 \cos \frac{2\pi}{4N}(2n+1) \quad n = 0, 1, \dots, \frac{N}{2} - 1 \quad (8)$$

Figure out $v(n)$'s DCT transform $V(k)$:

$$V(k) = \sum_{n=0}^{\frac{N}{2}-1} v(n) \cos \frac{2\pi}{2N} k(2n+1) \quad k = 0, 1, \dots, \frac{N}{2} - 1 \quad (9)$$

The $X(2k+1)$ can be derived from $V(k)$ and $X(2k-1)$:

$$X(1) = \frac{1}{2} V(0) \quad (10)$$

$$X(3) = V(1) - X(1) \quad (11)$$

$$X(5) = V(2) - X(3) \quad (12)$$

.....

$$X(N-1) = V\left(\frac{N}{2}-1\right) - X(N-3) \quad (13)$$

The algorithm flow is illustrated in Figure 8.

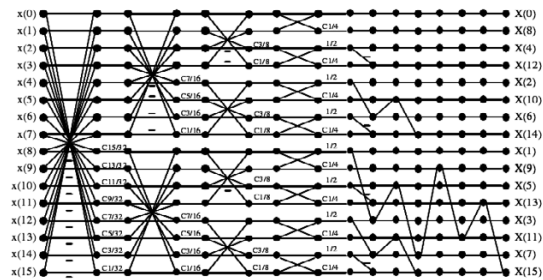


Fig. 8. Fast DCT algorithm

The operational complexity expressed in formula (14) and (15) is low, compared with FFT's operational complexity in real operation [8] [9] that can be expressed by (16) and (17):

$$\mu_m(N) = \frac{N}{2} \cdot \log_2 N \quad (14)$$

$$\mu_a(N) = \frac{N}{2} \cdot (3 \log_2 N - 2) + 1 \quad (15)$$

$$\mu_{m_FFT}(N) = 4 \cdot \frac{N}{2} \log_2 N \quad (16)$$

$$\mu_{a_FFT}(N) = 2 \cdot N \log_2 N \quad (17)$$

The DCT takes less computation time than the FFT does. Although, we use $N/2$ length FFT to calculate the N length DCT, this algorithm is still competitive.

In the frequency domain, Blackman window is applied to implement the filter. The Blackman window is defined by:

$$w(n+1) = 0.35875 + 0.48829 \cos\left(\frac{2\pi}{N}n\right) + 0.14128 \cos\left(\frac{2\pi}{N}2n\right) + 0.01168 \cos\left(\frac{2\pi}{N}3n\right) \quad N=400, \quad n = 0, 1, \dots, \frac{N}{2} \quad (18)$$

Here $X(k)$ is the signal sequence's DCT transform, and the filter is defined by:

$$X(k) = \begin{cases} X(k) \cdot w(k), & k \leq 201 \\ 0, & k > 201 \end{cases} \quad (19)$$

The 3db bandwidth of this filter is around 0.068π .

In order to evaluate this filter we generate a similar signal with 10% noise added. Figure 9 shows the effect of the filter.

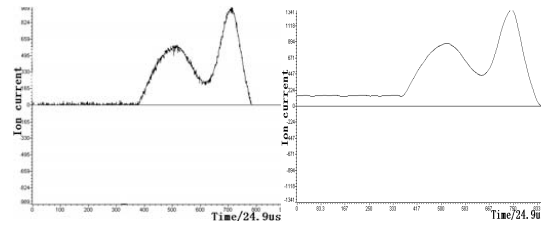


Fig. 9. Signal before filtering and after filtering

4.2. Smoothness

Here, a 9-point cubic smooth algorithm is applied in the formula of:

$$x(i) = [59 \cdot x(i) + 54 \cdot (x(i-1) + x(i+1)) + 39 \cdot (x(i-2) + x(i+2)) + 14 \cdot (x(i-3) + x(i+3)) - 21 \cdot (x(i-4) + x(i+4))] / 231 \quad (20)$$

We use the following expression to generate a signal and add a noise of 10% to simulate the ion signal with 3 peaks at 2, 5 and 6. The Figure 10 is the result after filtering and smoothness.

$$y = 5 + 1./((100 \cdot (t-2)^2 + 2) + 2./((100 \cdot (t-6)^2 + 4) + 10./((t-5)^2 + 4)) \quad (21)$$

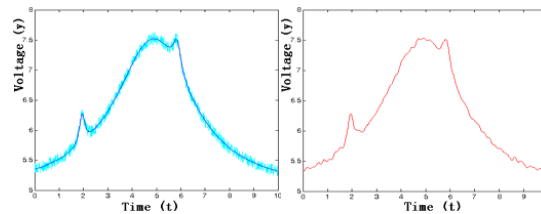


Fig. 10. Original signal and the signal after filtering and smoothness

4.3. Background subtracting

Many methods exist for background subtraction, each with different strengths and weaknesses in terms of performance and computational requirements. Here the background subtraction is being implemented on the hardware—the TMS320F28335, for real-time application, thus, the low-medium complexity, using the frame difference and approximate median method, is chosen.

Twenty points from the sampled signal sequences are taken:

$$bg(i) = mdata((i-1) \cdot itv) \quad (22)$$

Here, 'mdata' is the signal sequence after smoothness.

$$\text{If } \text{bg}(i) > (\text{bg}(i-1) + \text{bg}(i+1)) / 2, \quad (23)$$

$$\text{Then, } \text{bg}(i) = (\text{bg}(i-1) + \text{bg}(i+1)) / 2. \quad (24)$$

We calculate the background signal in this way for 10 times, and then subtract the background from the ion signal sequence.

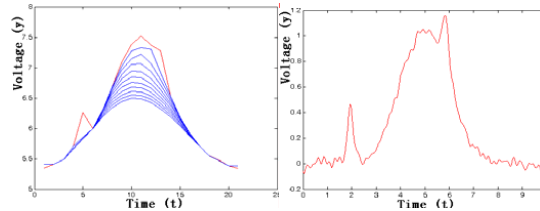


Fig. 11. Subtracting background from signal

4.4. Denoise

Before the de-noising implementation, the average and standard deviation of the noise are estimated. At the beginning, we suppose that the $\sigma = 100$, (that is big enough), assuming the points below $2.2 * \sigma$ are noise, then, we can calculate the standard deviation of noise again. Refresh the σ , and do it once again. After 10 times' calculate, we can roughly estimate the standard deviation and the average of the noise. We subtract the (average $\pm \sigma$) from signal. And the σ illuminates the strength of the noise, the true peaks will be selected according to the σ in the following peaks searching.

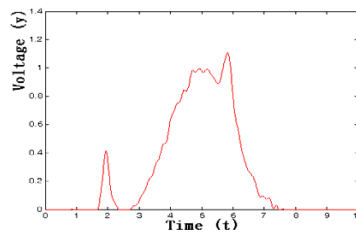


Fig. 12. De-noising

5. IMS SIGNAL PEAK SEARCHING

As we see in the Figure 12, there are many small peaks existed with the true signal peaks due to the mixture of various noise. A relative simple but effective algorithm can be applied to pick out the true peaks and ignore the false peaks.

First of all, we figure out all the half peaks and full peaks including the true and the false peaks with the rule that the first derivative equals to zero and the second derivative is less than zero. (That have been marked with “ \uparrow ” in Figure 13 (A)). At the same time we also find out all the valleys with the rule that the first derivative equals to zero and the second derivative is greater than zero. (That have been marked with “ \downarrow ” in Figure 13 (A)).

Secondly, re-search the peaks we have already figured out to find out the lowest valley between two peaks and calculate the height of the peaks. If the height between previous peak and the lowest valley is greater than 2.5σ , we consider that this previous peak has an effective back-half-peak, if there is an effective front-half-peak in front, we take this two half-peaks into one effective full-peak, we consider this a true full-peak which is marked by “ \uparrow ” as

shown in the Figure 13 (B). otherwise, if there is no effective front-half-peak in front, we consider this back-half-peak as a true independent half-peak which is marked by “↓” in the Figure 13 (B).

Continuously in the same way, if the height between posterior peak and the lowest valley is greater than 2.5σ , we consider that this posterior peak has an effective front-half-peak, if there is an effective front-half-peak in front, we consider the front-half-peak in front as a true independent half-peak which is marked by “↓” in the Figure 13 (B). Therefore, the true peaks in the ion signal are identified and the false peaks brought by the noise are ignored. From the Figure 13 (B) we can see the peaks at the positions of 2, 5, 6 defined in the formula (21) are identified as true peaks.

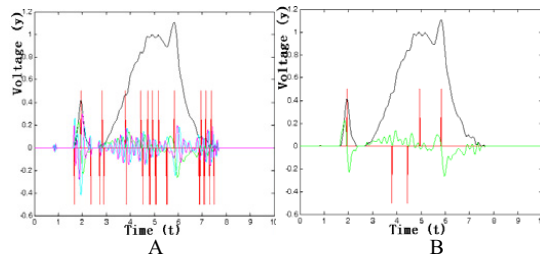


Fig. 13. Peaks searching

6. DISCUSSION AND CONCLUSION

We have successfully implemented a DSP based back-end platform with functionalities of signal acquisition, filtering, de-noising, background subtraction, peaks searching, and feedback control, etc, for a home-made portable IMS instrument. It is based on Spectrum Digital Inc's eZdsp™ F28335 board [10].

The system clock (CLK) for F28335 is 150 MHz. We took comprehensive experimental testing of the system and found that the DCT operation takes 931,961 CLKs. All other pre-processing steps and peak searching take 2,571,094 CLKs if there is no true peak in the signal, and 2,236,063 CLKs when three true peaks existed. The frame difference and approximate median method for background subtraction can significantly increase accuracy for not much more computation. Peak searching time is related to the shape of the signal. The larger rate the signal over 3σ of the noise possesses, the fewer time the operation takes, mainly because of the de-noise operation.

All those processing and operations on the DSP board generally take about 25ms, the frame rate of the spectrum, that means it satisfies the requirements of IMS instrument for real-time detection and monitoring.

7. ACKNOWLEDGEMENT

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